2,2,4-Trimethyl-1,3-pentanediol
144-19-4 | DTXSID8027113

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.69e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.39e-01

Confidence level: 8.33e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
2-(2-Butoxyethoxy)ethanol	Butane, 1,1'-[methylenebis(oxy)]bis-	1-Butoxy-2-propanol
Measured: 7.44e-11	**Measured:** 3.39e-11	**Measured:** 3.76e-11
Predicted: 5.15e-11	**Predicted:** 3.22e-11	**Predicted:** 3.73e-11